

Nonlinear Impurity in a Lattice: Dispersion Effects

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Abstract

We examine the bound state(s) associated with a single cubic nonlinear impurity, in a one-dimensional tight-binding lattice, where hopping to first- and second nearest neighbors is allowed. The model is solved in closed form *via* the use of the appropriate lattice Green function and a phase diagram is obtained showing the number of bound states as a function of nonlinearity strength and the ratio of second to first nearest-neighbor hopping parameters. Surprisingly, a finite amount of hopping to second nearest neighbors helps the formation of a bound state at smaller (even vanishingly small) nonlinearity values. As a consequence, the selftrapping transition can also be tuned to occur at relatively small nonlinearity strength, by this increase in the lattice dispersion.

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The effects of impurities on the transport properties of materials continues to be an interesting subject. When the concentration of impurities inside a material is finite, we speak of a disordered system. In one dimensional systems, this disorder gives rise to the well-known phenomenon of Anderson localization, where all states acquire a finite localization length. This precludes any amount of transport in the system. Economou and coworkers[1] have argued that there exist a correspondence between the property that, in dimensions smaller or equal to two, all states of a disordered system are localized, and the property that an isolated impurity can always trap a particle. More recently, the problem of *nonlinear* impurities have received considerable attention. In a condensed matter context, they appear in strongly coupled electron–vibration systems, when the vibrational degrees of freedom have the ability of adapting quickly to the presence of the electron, giving rise to polaronic behavior[2]. Nonlinear impurities appear also in other fields, such as nonlinear optics. For instance, an array of linear waveguides containing a single or several nonlinear, Kerr-like guides. The transversal dynamics describing the energy exchange among waveguides is formally identical to the dynamics of an excitation propagating in a linear tight-binding lattice in the presence of one or more nonlinear impurities[3].

In systems where an electron (or excitation) is propagating while strongly interacting with vibrational degrees of freedom, an “effective” nonlinear evolution equation for the electron can be obtained, under the assumption that the vibrations adapt instantly to the presence of the electron[2]. This equation, known as the Discrete Nonlinear Schrödinger (DNLS) equation, has the form:

$$i \left(\frac{dC_{\mathbf{n}}}{dt} \right) = V \sum_{\mathbf{n},\mathbf{n}'} C_{\mathbf{n}'} - \chi_{\mathbf{n}} |C_{\mathbf{n}}|^2 C_{\mathbf{n}} \quad (\hbar \equiv 1), \quad (1)$$

where $C_{\mathbf{n}}$ is the probability amplitude of finding the electron on lattice site \mathbf{n} at time t , V is the nearest-neighbor hopping parameter and $\chi_{\mathbf{n}}$ is the nonlinearity parameter at site \mathbf{n} proportional to the square of the electron–vibration coupling. In the conventional DNLS equation, the sum in (1) is restricted to nearest-neighbors (n.n.).

For the case of a single nonlinear impurity in a onedimensional lattice ($\chi_n = \delta_{n,0} \chi$), we have obtained in a previous work[4] its bound state analytically, *via* lattice Green functions, and have shown that a bound state

is possible provided $|\chi/2V| > 1$. This result deviated markedly from the well-known linear impurity case where, a bound state exists for any impurity strength. The extension to an impurity of arbitrary nonlinear exponent α (i.e., $|C_{\mathbf{n}}|^\alpha$ instead of $|C_{\mathbf{n}}|^2$ in (1)), revealed[5, 6] that for $\alpha < 2$ there is always a bound state for any finite χ/V . At $\alpha = 2$ (the standard DNLS case) there is one bound state for $|\chi/2V| > 1$, while for $\alpha > 2$ there is a critical curve in χ - α space, below which there is no bound state, while above it, there are two bound states. On the critical curve, there is a single bound state.

When this nonlinear impurity is embedded in a square lattice[7], the χ - α bound state phase diagram shows a single curve separating two regimes. Below the curve, there are no bound states; on the curve there is a single bound state, while above the curve there are two bound states. One of these become more localized upon increment of the nonlinearity parameter while the other becomes more delocalized. Bound states for single nonlinear impurities have also been computed for other systems, including a Cayley tree[8], a triangular lattice[10] and a cubic lattice[9, 10].

In all the studies above, only dispersion to first nearest-neighbors has been considered. For systems with long-range dispersion, a continuum-like approximation that employs a nonlocal nonlinear Schrödinger equation has been proposed[11]. For the case of a discrete system with a hopping parameter of the form $V_{nm} = V/|n - m|^s$, another study[12] followed a variational approach, based on a plausible *ansatz* for the localized state. Among other things, they found that there is a critical s_{cr} such that all dispersive interactions decreasing faster than $r^{-s_{cr}}$ lead to similar qualitative behavior as the DNLS with only nearest neighbor transfer. In this work we solve in closed form *via* Green functions, the case of a single DNLS impurity in a tight-binding lattice, including hopping to first and second nearest-neighbors. Since the phenomenon of selftrapping is the result of the quantum struggle between the tendency to spread (dispersion) and the tendency to localize (nonlinearity), one might surmise that any increase in dispersion will have the simple effect of increasing the nonlinearity needed to selftrap. However as we will see, this is not necessarily the case and a small increment in dispersion can actually favor the formation of a bound state at smaller nonlinearity

strength.

1 Onedimensional lattice with dispersion

Let us consider the problem of determining the existence of bound states and dynamic selftrapping characteristics for an electron (or an excitation) moving on a onedimensional dispersive lattice with hopping up to second nearest-neighbors, which contains a single DNLS impurity at the origin $n = 0$. The DNLS equation (1) reduces to

$$i \left(\frac{dC_n}{dt} \right) = V_1(C_{n+1} + C_{n-1}) + V_2(C_{n+2} + C_{n-2}) - \chi |C_0|^2 C_0 \delta_{n,0}. \quad (2)$$

For stationary states, one puts $C_n(t) = \exp(-iEt) \phi_n$, obtaining

$$E \phi_n = V_1(\phi_{n+1} + \phi_{n-1}) + V_2(\phi_{n+2} + \phi_{n-2}) - \chi |\phi_0|^2 \phi_0 \delta_{n,0}. \quad (3)$$

The Hamiltonian that gives rise to (2) is

$$\tilde{H} = \tilde{H}_0 + \tilde{H}_1, \quad (4)$$

where

$$\tilde{H}_0 = V_1 \sum_n (|n\rangle\langle n+1| + |n+1\rangle\langle n|) + V_2 \sum_n (|n\rangle\langle n+2| + |n+2\rangle\langle n|) \quad (5)$$

and

$$\tilde{H}_1 = -\chi |\phi_0|^2 |0\rangle\langle 0|. \quad (6)$$

The $\{|n\rangle\}$ represent Wannier electronic states and $V_1(V_2)$ is the nearest (next-to-nearest) neighbor transfer matrix element. In the absence of impurity, the energy band is given by

$$E(k) = 2 V_1 \cos(k) + 2 V_2 \cos(2k). \quad (7)$$

A simple analysis shows that, for positive V_2/V_1 , the upper and lower band edges obey

$$E_{max} = 2(V_1 + V_2) \quad (8)$$

$$E_{min} = \begin{cases} -2(V_1 - V_2) & V_2/V_1 < 1/4 \\ -(V_1^2/4V_2) - 2V_2 & V_2/V_1 > 1/4 \end{cases} \quad (9)$$

As a result, while the upper edge always increase linearly with V_2 , the lower edge first decreases (in magnitude), reaching a minimum value of $2(1 - (1/\sqrt{8}))V_1 \approx 1.29V_1$ at $V_2 = (1/\sqrt{8})V_1$. Afterwards, the lower edge increases in magnitude with V_2 . At large V_2 , this increase will be almost linear. These features will of importance in the next section, where we determine the position of the impurity bound state(s).

The formalism of lattice Green functions is particularly suitable for the problem of determining the bound state(s). First, we normalize all energies by V_1 and define: $z \equiv E/V_1$, $H \equiv \tilde{H}/V_1$, $\gamma \equiv \chi/V_1$ and $\delta \equiv V_2/V_1$. The dimensionless lattice Green function $SG = 1/(z-H)$ can be formally expanded as[14]

$$G = G^{(0)} + G^{(0)}H_1G^{(0)} + G^{(0)}H_1G^{(0)}H_1G^{(0)} + \dots \quad (10)$$

where $G^{(0)}$ is the unperturbed ($\gamma = 0$) Green function and $H_1 = -\gamma|\phi_0|^2 |0\rangle\langle 0|$. The sum in Eq.(10) can be carried out exactly to yield

$$G_{mn} = G_{mn}^{(0)} - \frac{\gamma|\phi_0|^2 G_{m0}^{(0)} G_{0n}^{(0)}}{1 + \gamma|\phi_0|^2 G_{00}^{(0)}}. \quad (11)$$

where $G_{mn} = \langle m|G|n \rangle$ and

$$G_{mn}^{(0)}(z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\phi \frac{\exp[i\phi(m-n)]}{[z - \cos(\phi) - \delta \cos(2\phi)]}. \quad (12)$$

whose evaluation in closed form is done in the *Appendix*.

1.1 Bound States

The energy of the bound state(s), z_b is obtained from the poles of G_{mn} , *i.e.*, by solving $1 = -\gamma|\phi_0^{(b)}|^2 G_{00}^{(0)}$. The bound state amplitudes $\phi_n^{(b)}$ are obtained from the residues of $G_{mn}(z)$ at $z = z_b$. In particular,

$$|\phi_0^{(b)}|^2 = \text{Res}\{G_{00}(z)\}_{z=z_b} = -\frac{G_{00}^{(0)2}(z_b)}{G_{00}^{(0)'}(z_b)} \quad (13)$$

Inserting this in the bound state energy equation leads to

$$\frac{1}{\gamma} = \frac{G_{00}^{(0)3}(z_b)}{G_{00}^{(0)'}(z_b)}. \quad (14)$$

Now, as the reader can easily verify using (14) and (12), changing both, the sign of χ/V_1 and the sign of V_2/V_1 has the effect of changing the sign of the corresponding eigenvalue. Thus, for a complete parameter space examination of all the possible eigenvalues, we only need to consider a fixed sign for V_2/V_1 (say, positive) and the two possible signs of χ/V_1 .

Figure 1 shows the left- and right-hand side of (14) for several (positive) values of δ . When $\gamma > 0$ (Fig. 1a) and as δ increases from zero, the RHS of (14) moves towards the origin and increases its height, until δ reaches $1/4$, where the height diverges. Further increase in δ decreases the height of the curves, but they continue to approach the origin until $\delta = 1/\sqrt{8}$. Afterwards, the curves move away from the origin while their heights continue to decrease. For the case of $\gamma < 0$ (Fig. 1b), the situation is quite different: For a given δ value, there is a minimum $|\gamma_a|$ at which there is a bound state. Further increase in $|\gamma|$ creates two bound states, one of which will ultimately disappear at a further finite $|\gamma_b|$ value, leaving only a single bound state.

Figure 2 displays a phase diagram in nonlinearity–dispersion space showing the number of bound state(s). For positive nonlinearity, the critical curve separating the region with no bound states from the region with one bound state, decreases with increasing δ and reaches zero at $\delta = 1/4$. Afterwards, it increases monotonically with further dispersion. Thus, there is a finite dispersion interval, $0 < \delta < 1/4$ where, contrary to what might be expected, an increase in dispersion actually *reduces* the nonlinearity needed to create a bound state. This can also be seen in Fig. 3a, which shows the bound state energy as a function of (positive) nonlinearity, for several values of dispersion δ . This reduction in nonlinearity needed to sustain a bound state is, of course due to the reduction in the width of the negative portion of the band with a small positive dispersion, and thus, it has a *linear* origin. In the negative nonlinearity sector, we have in Fig.2 two critical curves separating regions with no bound states, two bound states and one bound state. Here, an increase in dispersion, causes a corresponding increase in the minimum nonlinearity needed for the creation of a bound state(s). This is correlated with the fact that the width of the positive portion of the band always increases linearly with δ . Figure 3b, shows the bound state energy as a function of nonlinearity, for negative γ . Here, for a given value of δ , there exists a critical

nonlinearity value γ_a for which there is a bound state, with energy outside the band. Further increase in nonlinearity creates two bound states, one of which increases its energy monotonically with nonlinearity while the other state decreases its energy towards the band, reaching it at a finite nonlinearity value γ_b . As Fig. 4 shows, in the regime with two bound states, as the magnitude of the nonlinearity is increased, one of the states becomes more localized on the impurity site, while the other becomes more delocalized, ultimately disappearing into the continuum at a finite nonlinearity value.

1.2 Transmission across the impurity

Inside the band, $z_{min}(\delta) < z < z_{max}(\delta)$ (see (8) and (9)), all states are extended and given by[14]

$$|\psi\rangle = |k\rangle + G^{(0)+} T^+(z) |k\rangle, \quad (15)$$

where $|k\rangle$ is a plane wave and the scattering-matrix T is

$$T = H_1 + H_1 G^{(0)} H_1 + H_1 G^{(0)} H_1 G^{(0)} H_1 + \dots \quad (16)$$

This can be summed exactly, to yield

$$T = \frac{-\gamma |C_0|^2 |0\rangle \langle 0|}{1 + \gamma |C_0|^2 G_{00}^{(0)}}. \quad (17)$$

With this, we can compute the scattering amplitude at any site n . In particular, the scattering amplitude at the *impurity site* $C_0 = \langle 0|\Psi\rangle$ is

$$C_0 = \langle 0|k\rangle - \frac{\gamma |C_0|^2 \langle 0|G^{(0)+}(z)|0\rangle \langle 0|k\rangle}{1 + \gamma |C_0|^2 G_{00}^{(0)}}. \quad (18)$$

The transmission coefficient is then given by the probability at the impurity site, $t = |C_0|^2$. From (18), we have

$$t = \frac{1}{|1 + \gamma t G_{00}^{(0)}|^2} = \frac{1}{1 + \gamma^2 t^2 \text{Im}[G_{00}^{(0)}(z)]^2} \quad (19)$$

which leads to the cubic equation: $\gamma^2 t^3 \text{Im}[G_{00}^{(0)}(z)]^2 + t - 1 = 0$. This is invariant under $\gamma \rightarrow -\gamma$, implying that the transmission does not depend on

the sign of the nonlinearity parameter. The physical solution for t is

$$t = \frac{-2 \cdot 6^{\frac{1}{3}} + \left(18 \gamma \text{Im}[G_{00}^{(0)}(z)] + 2 \sqrt{3} \sqrt{4 + 27 \gamma^2 \text{Im}[G_{00}^{(0)}(z)]^2}\right)^{\frac{2}{3}}}{2 \cdot 3^{\frac{2}{3}} \gamma \text{Im}[G_{00}^{(0)}(z)] \left(9 \gamma \text{Im}[G_{00}^{(0)}(z)] + \sqrt{3} \sqrt{4 + 27 \gamma^2 \text{Im}[G_{00}^{(0)}(z)]^2}\right)^{\frac{1}{3}}}. \quad (20)$$

The specific form of $\text{Im}[G_{00}^{(0)}(z)]$ in our case, is given in closed form in the *Appendix*. Figure 5 shows several transmission curves as functions of the plane waves dimensionless energy z , for several different ratios δ . The most remarkable new feature is the appearance of an abrupt “dip” on the transmission near the lower edge of the band at $\delta \sim 0.4$. As δ increases further, the “dip” moves to the right and eventually (not shown) approaches the upper band edge and merges with it. This “dip” is related to the creation of a secondary “branch” in $\text{Im}[G_{00}^{(0)}(z)]$, as shown in Fig. B of the *Appendix*.

1.3 Dynamic Selftrapping

We place the electron at the impurity site at $t = 0$ and observe its time evolution, according to Eq.(2). The observable of interest here is the long-time average probability of finding the electron on the initial site after a relatively long time T :

$$P_0 = \lim_{T \rightarrow \infty} (1/T) \int_0^T |C_0(t)|^2 dt, \quad |C_0(0)| = 1. \quad (21)$$

By using the transformation $C_n \rightarrow (-1)^n C_n$, that leaves $|C_n|^2$ invariant, the reader can verify that changing $V_2 \rightarrow -V_2$ and $\chi \rightarrow -\chi$, transforms (2) into its complex conjugate. Thus, for our completely localized real initial condition $C_0(0) = 1$, the observable P_0 is invariant under the transformation. Therefore, for a complete parameter study, it is enough to consider a positive V_2 (or δ) and the two possible signs for the anharmonicity χ (or γ).

We use a fourth-order Runge-Kutta numerical scheme, whose accuracy is monitored through total probability conservation: $1 = \sum_n |C_n(t)|^2$. To avoid undesired boundary effects, a self-expanding lattice is used[13]. Figure 6 shows P_0 as a function of (positive) nonlinearity parameter γ , for several different dispersion δ values. As anticipated from the bound state results, an increase of dispersion reduces the critical nonlinearity for the onset of

selftrapping. The minimum threshold occurs around $\delta \approx 0.3$. In the immediate vicinity of this value, the selftrapping transition also seems to lose some sharpness. Subsequent increase in δ increases the critical nonlinearity γ_c again and restores sharpness to the P_0 curve. At $\delta \approx 1$, the P_0 curve almost coincides with the $\delta = 0$ case. Thereafter, γ_c increases in an almost linear fashion with δ . For the case of a negative nonlinearity parameter (not shown), the critical nonlinearity always increases monotonically with dispersion. As explained above, this case corresponds also to $\gamma > 0, \delta < 0$.

2 Discussion

We have examined the conditions for the formation of a bound state at a nonlinear impurity site, in a onedimensional linear lattice with hopping to first and second nearest-neighbors. The formalism employed lattice Green functions, which have been evaluated in closed form for our system. We found that this increment in dispersion can actually favor the formation of a bound state at smaller nonlinearity strength. As a consequence, the onset of dynamical selftrapping at the impurity site can also be shifted to lower nonlinearity thresholds. This tuning effect could have some impact on the design of completely nonlinear optical or solid nanostructures, where one is interested in static (“selftrapped”) or mobile discrete nonlinear excitations (“discrete solitons”). In the former, one is interested in achieving abrupt selftrapping at relatively low nonlinearity (or input power) parameter values; in the latter, the probability profile corresponding to an impurity bound state, could be useful as an initial condition for the launch of a discrete soliton, which can carry energy across a nonlinear fiber array from a given guide to another, distant one[15].

3 Acknowledgments

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4 APPENDIX: THE LATTICE GREEN FUNCTION

The dimensionless lattice Green function for our tight-binding chain including dispersion up to second nearest-neighbors is

$$G_{mn}^{(0)}(z) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\phi \frac{\exp[i\phi(m-n)]}{[z - \cos(\phi) - \delta \cos(2\phi)]}. \quad (22)$$

We follow the usual method[1] of transforming (22) to an integral over a complex variable w along the unit circle. Thus, we have

$$G_{mn}^{(0)}(z) = -\frac{1}{2\pi i} \oint \frac{dw w^{|l-m|+1}}{\delta w^4 + w^3 - w^2 z + w + \delta} \quad (23)$$

The roots of $\delta w^4 + w^3 - w^2 z + w + \delta = 0$ are given by

$$\begin{aligned} z_1 &= \frac{-1 + \delta \gamma_1(z) - \sqrt{2}\sqrt{\gamma_2(z) - \delta \gamma_1(z)}}{4\delta} \\ z_2 &= \frac{-1 - \delta \gamma_1(z) + \sqrt{2}\sqrt{\gamma_2(z) + \delta \gamma_1(z)}}{4\delta} \\ z_3 &= \frac{-(1 + \delta \gamma_1(z) + \sqrt{2}\sqrt{\gamma_2(z) + \delta \gamma_1(z)})}{4\delta} \\ z_4 &= \frac{-1 + \delta \gamma_1(z) + \sqrt{2}\sqrt{\gamma_2(z) - \delta \gamma_1(z)}}{4\delta} \end{aligned}$$

where $\gamma_1(z) \equiv \sqrt{8 + (1/\delta^2) + (4z/\delta)}$ and $\gamma_2(z) \equiv 1 - 4\delta^2 + 2\delta z$. Only the poles contained inside the unit circle contribute to the integral. Thus,

$$\begin{aligned} |z_1| < 1 &\Rightarrow 2(1 + \delta) < z < \infty \\ |z_2| < 1 &\Rightarrow \begin{cases} -\infty < z < \infty, & \delta < 1/4 \\ -\infty < z < -1/(4\delta) - 2\delta & \text{and } 2(\delta - 1) < z < \infty, & \delta > 1/4 \end{cases} \\ |z_3| > 1 &\Rightarrow \text{no contribution} \\ |z_4| < 1 &\Rightarrow \begin{cases} -\infty < z < -2(1 - \delta), & \delta < 1/4 \\ -\infty < z < -1/(4\delta) - 2\delta, & \delta > 1/4 \end{cases} \end{aligned}$$

Using the above, we can express $G_{lm}^{(0)}(z)$ as

$$G_{lm}^{(0)}(z) = -\frac{1}{2\pi\delta} \oint \frac{dw w^{|l-m|+1}}{\delta(w - z_1)(w - z_2)(w - z_3)(w - z_4)} \quad (24)$$

$$\begin{aligned}
&= -\frac{\Theta[z - (2(1 + \delta))] z_1^{|l-m|+1}}{\delta(z_1 - z_2)(z_1 - z_3)(z_1 - z_4)} + \\
&\quad - \frac{[\Theta((1/4) - \delta) + \Theta(\delta - (1/4))][\Theta(-1/(4\delta - 2\delta - 2z)) + \Theta(z - 2(\delta - 1))]}{\delta(z_2 - z_1)(z_2 - z_3)(z_2 - z_4)} z_2^{|l-m|+1} + \\
&\quad - \frac{[\Theta((1/4) - \delta)\Theta(-2(1 - \delta) - z) + \Theta(\delta - (1/4))\Theta(-1/(4\delta) - 2\delta - 2z)] z_4^{|l-m|+1}}{\delta(z_4 - z_1)(z_4 - z_2)(z_4 - z_3)} \quad (25)
\end{aligned}$$

After some tedious algebra, we find for the real and imaginary parts of the diagonal Green function:

$$\text{Re}[G_{00}^{(0)}(z)] = \begin{cases} 2\sqrt{2}\delta [(\gamma_1\delta + \gamma_2)\sqrt{1 - \delta(4\delta - 2z + \gamma_1)} + \\ (\gamma_1\delta - \gamma_2)\sqrt{1 + \delta(-4\delta + 2z + \gamma_1)}]^{-1} & z > z_{\max}(\delta) \\ - 2\sqrt{2}\delta [(\gamma_1\delta + \gamma_2)\sqrt{1 - \delta(4\delta - 2z + \gamma_1)} - \\ (\gamma_1\delta - \gamma_2)\sqrt{1 + \delta(-4\delta + 2z + \gamma_1)}]^{-1} & z < z_{\min}(\delta) \\ 0 & \text{otherwise} \end{cases} \quad (26)$$

where,

$$z_{\min}(\delta) = \begin{cases} -2(1 - \delta) & \delta < 1/4 \\ -1/(4\delta) - 2\delta & \delta > 1/4 \end{cases}$$

and

$$z_{\max} = 2(1 + \delta)$$

$$\begin{aligned}
\text{Im}[G_{00}^{(0)}(z)] &= \frac{\Theta((1/4) - \delta)[\Theta(z - 2(\delta - 1)) - \Theta(z - 2(1 + \delta))]}{2\sqrt{1 - d_1(z)^2}|1 + 4\delta d_1(z)|} + \\
&\quad \frac{\Theta(\delta - (1/4))[\Theta(z + (1/(4\delta)) + 2\delta) - \Theta(z - 2(1 + \delta))]}{2\sqrt{1 - d_1(z)^2}|1 + 4\delta d_1(z)|} + \\
&\quad \frac{\Theta(\delta - (1/4))[\Theta(z + (1/(4\delta)) + 2\delta) - \Theta(z - 2(\delta - 1))]}{2\sqrt{1 - d_2(z)^2}|1 + 4\delta d_2(z)|} \quad (27)
\end{aligned}$$

where, $d_1(z) \equiv (1/4)\delta(-1 + \sqrt{1 + 8\delta(\delta + (z/2))})$ and $d_2(z) \equiv (1/4)\delta(-1 - \sqrt{1 + 8\delta(\delta + (z/2))})$.

Figures A and B, show $\text{Re}[G_{00}^{(0)}(z)]$ and $\text{Im}[G_{00}^{(0)}(z)]$, respectively for different values of dispersion δ .

References

- [1] E.N. Economou and C.M. Soukoulis, Phys. Rev. B **28**, 1093 (1983); E. N. Economou, C.M. Soukoulis and A.D. Zdetsis, *ibid.* **30**, 1686 (1984).
- [2] See, for instance, D. Chen, M. I. Molina and G. P. Tsironis, J. Phys.: Condens. Matter **5**, 8689 (1993); D. Chen, M. I. Molina and G. P. Tsironis, J. Phys.: Condens. Matter **8**, 6917 (1996).
- [3] See, for instance, G. P. Tsironis, W. D. Deering and M. I. Molina, Physica D **68**, 135 (1993) and references therein.
- [4] M. I. Molina and G. P. Tsironis, Phys. Rev. B **47**, 15330 (1993);
- [5] G. P. Tsironis, M. I. Molina and D. Hennig, Phys. Rev. E **50**, 2365 (1994).
- [6] M.I. Molina in *Topics in Theoretical Physics*, edited by V.C. Aguilera-Navarro, D. Galletti, B.M. Pimentel and L. Tomio, (IFT, Sao Paulo, 1996); M.I. Molina, Phys. Rev. B **60**, 2276 (1999).
- [7] M.I. Molina, Phys. Rev. B **60**, 2276 (1999); K. M. Ng, Y.Y. Yiu and P.M. Hui, Solid State Commun. **95**, 801 (1995).
- [8] B. C. Gupta and S. B. Lee , Phys. Rev. B **63**, 144302 (2001).
- [9] Y. Y. Yiu, K. M. Ng and P. M. Hui, Phys. Lett. A **200**, 325 (1995)
- [10] C. A. Bustamante and M. I. Molina, Phys. Rev. B **62**, 15287 (2000).
- [11] Yu. B. Gaididei, S. F. Mingaleev, P. L. Christiansen and K. Ø. Rasmussen, Phys. Lett. A **222**, 152 (1996).
- [12] K. Ø. Rasmussen, P. L. Christiansen, M. Johansson, Yu. B. Gaididei and S. F. Mingaleev, Physica D **113**, 134 (1998).
- [13] M.I. Molina and G.P. Tsironis, Phys. Rev. Lett. **73**, 464 (1994).
- [14] E.N. Economou, *Green's Functions in Quantum Physics*, Springer Series in Solid State Physics, Vol.7 (Springer-Verlag, Berlin, 1979).

- [15] W. Królikowski, U. Trutschel, M. Cronin-Golomb and C. Schmidt-Hattenberger, *Opt. Lett.* **19**, 320 (1994); W. Królikowski and Y. Kivshar, *J. Opt. Soc. Am.* **13**, 876 (1996).

Captions List

Fig.1 : Left-and-right hand side of the eigenenergy equation (14), for several dispersion δ values, for positive (a) and negative(b) nonlinearity.

Fig.2 : Bound state phase diagram in nonlinearity–dispersion space ($\gamma \equiv \chi/V_1, \delta \equiv V_2/V_1$)

Fig.3 : Bound state energy as a function of positive (a) and negative(b) nonlinearity, for several dispersion values.

Fig.4 : Probability at the impurity site as a function of nonlinearity, in the negative nonlinearity sector, for several dispersion values.

Fig.5: Transmission coefficient of plane waves across the nonlinear impurity as a function of the plane wave dimensionless energy, for several dispersion values.

Fig. 6: Long-time average probability of finding the electron on the impurity site, as a function of nonlinearity, for several different dispersion values. ($T = 203 V_1$)

Fig. A: Real part of the diagonal unperturbed Green function $G_{00}^{(0)}(z)$, for several dispersion values: 0 (a), 0.2(b), 0.4(c), 0.6 (d), 0.8 (e) and 1.0(e).

Fig. B: Same as in Fig. A, but for the imaginary part of $G_{00}^{(0)}(z)$.

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